Electronic structure of FeAl(1 1 0) using upgraded 6 m-TGM at CAMD

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Abstract

A new endstation has recently been commissioned at 6-m toroidal grating monochromator beamline to perform high-resolution photoemission studies in the photon energy range of 10–180 eV. The new endstation is equipped with Phoibos-150 analyzer with a channelplate and charge coupled device (CCD) camera readout to measure the kinetic energy of the electron and its emission angle simultaneously. The initial energy resolution test of the analyzer from He-I discharge lamp excited Argon 3p gas phase spectra reveals ∼20 meV full-width-half-maximum (FWHM).

With this new set-up, we have investigated the electronic structure of FeAl(1 1 0). Preferential sputtering of clean FeAl(1 1 0) surface results in depletion of Al in the near surface region. The surface forms reconstructed phases at different annealing temperature regions. The electronic structure of these phases is presented.

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1. Introduction

The fundamental significance of intermetallic alloy surfaces is their effect on physical and chemical properties such as corrosion resistance, oxidation, and catalytic activity. New materials displaying unprecedented properties can be attained by changing the stoichiometry of alloys. To modify and control these properties require a detailed understanding of the atomic and electronic structure of the alloys. Specifically, transition metal aluminides, e.g. NiAl, CoAl, and FeAl, have attracted considerable interest due to their unique properties such as high melting points, enhanced corrosion resistance, relatively low density, and utility as soft magnetic materials.

These transition metal aluminides, most notably NiAl, are ordered intermetallic alloys. Their surfaces are expected to be bulk terminated due to the strong interaction between the different atoms. FeAl also crystallizes in the CsCl structure, as other late transition metal aluminides do. Surprisingly, it has been reported by Graupner et al. [1,2] that, in contrast to NiAl(1 1 0) and CoAl(1 1 0) surface, FeAl(1 1 0) does not follow the trend of the late transition metal alloys.

2. Experimental procedure

The initial energy resolution tests of this analyzer were taken with a He-I discharge lamp used to excite Argon 3p emission lines. The Ar-3p\textsubscript{1/2} and Ar-3p\textsubscript{3/2} emissions at binding energies of 15.94 and 15.76 eV, respectively, are shown in Fig. 1. The inset of Fig. 1 shows the Gaussian fit of Ar-3p\textsubscript{3/2}, which reveals a FWHM of 23 meV. This measurement was taken with a 1 × 20 mm entrance slit size. The smallest entrance slit for this analyzer is 0.2 × 20 mm, and current work is underway to achieve the ultimate energy resolution which is expected to be ∼6 meV.

A variable temperature STM at CAMD made by the STM group at the University of Aarhus in Denmark was used to corroborate the electronic structure.
The FeAl(1 1 0) surface was cleaned by repeated cycles of sputtering at room temperature (Ne\(^+\) ions, 1.5 keV, 10 \(\mu\)A).

3. Atomic and electronic structure of FeAl

Sputtering the FeAl(1 1 0) crystal gives rise to a depletion of Al in the near surface region and the annealing of this surface promotes the diffusion of Al atoms from the bulk to the surface selvage. At 400°C, STM (Fig. 2(a)) and LEED measurements elucidate a bulk terminated surface structure. In the temperature range of 400–600°C, a significant rise of Al signal was obtained in the Auger electron spectrum [1], which indicates Al segregation to the near surface region. This higher Al concentration leads to an incommensurate structure on the surface. The STM image in Fig. 2(b) illustrates a quasi hexagonal overlayer from this high-temperature incommensurate phase. However, segregated Al atoms induce a strain field in the surface region. In order to reduce the strain field, the surface reconstructs as revealing a missing-row-like superstructure along the [0 0 1] direction at annealing temperatures of 600–800°C (Fig. 2(c)). At temperatures above 800°C a structural transition from the missing-row like superstructure to an incommensurate phase occurs. This result gives rise to the topmost concentration of Al to be 0.67 ± 0.06, corresponding to FeAl\(_2\) stoichiometry. The details of the atomic structure of this incommensurate phase are seen in the STM image in Fig. 2(d).

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**Fig. 1.** Ar-3p gas spectra excited by He-I discharge lamp (21.2 eV). The inset shows a FWHM of 23 meV for Ar-3p\(_{3/2}\) emission band.

**Fig. 2.** STM image of: (a) bulk terminated (7×7 nm\(^2\)), (b) incommensurate (5×5 nm\(^2\)), (c) missing-row like (20×20 nm\(^2\)), (d) incommensurate superstructures (15×15 nm\(^2\)) after annealing the crystal to 400, 600, 700 and 850°C, respectively.
The physical and chemical properties of the transition metal aluminides are facilitated by the interaction between Al sp and transition metal d-bands. The chemical bonding is affected by Al concentration changes, causing hybridization between the sp and d-bands. The charge transfer increases as the Al concentration increases in the alloy.

In normal emission from FeAl(110), the states having $\Sigma$ symmetry along the $\Gamma M$ symmetry line are probed. The $\Sigma_1$ band in the calculated band structure along this line is s-like. The next $\Sigma_1$ band is a mixture of s and d-states. The bands from the Fermi level to 2.75 eV comprise mostly Fe d-bands.

The segregation of Al atoms to the surface after annealing at higher temperatures modifies the surface potential. This modification results in an increased hybridization between the Fe d and Al p-states. The photoemission spectra in Fig. 3 compare the bulk terminated surface with other reconstructed surfaces for a photon energy of 60 eV along the $A_\perp[001]$ direction. The major difference between the spectra is the appearance of a new feature near the Fermi level ($\sim 0.3$ eV) on the photoemission spectra of the reconstructed phases. We believe that this band is the consequence of the hybridization of the Fe d-band with the Al p-band. This state is an induced state due to hybridization phenomenon, and the reduction of the symmetry resulting from the reconstruction and the modified surface charge density.

4. Conclusion

The geometric and electronic structure of FeAl(110) intermetallic alloy has been investigated by STM and ARPES. Preferential sputtering results in Al depletion in the near surface region and subsequent annealing promotes surface segregation of Al and gives rise to the new reconstructed phases on the surface. The increased density of state near Fermi level for the reconstructed phases is believed to be due to hybridization between the Fe d-band and Al p-band.

References